Fluid-Fluid Interfacial Tension of Binary Mixtures from Perturbative Methods

Francisco José Martínez-Ruiz, Jesús Algaba-Fernández, Ana Villegas-Páez, A. Ignacio Moreno-Ventas Bravo and Felipe J. Blas [C, S]

Universidad de Huelva, Departamento de Física Aplicada, Huelva, Spain

felipe@uhu.es

Molecular interactions, including molecular size and dispersive energy, determine critically the delicate interplay between surface and bulk contributions to the free energy. During the last decade there has been an intensive and increasingly development of the Monte Carlo methods for determining fluid-fluid interfacial properties of complex liquids. Although the traditional method for determining the surface tension is the virial method or mechanical route, a number of new strategies have been proposed in last years, including the Test-Area, Wandering Interface Method, or Expanded Ensemble, which allow the determination of the interfacial tension easily and in an elegant way. In this work we use and generalize some of these methods to determine the behavior of the interfacial properties of binary mixtures of molecules that interact through spherical intermolecular potentials. We have determined the behavior of the surface tension, and other thermodynamic and structural properties such as density profile, critical temperature and density, vapour pressure, and interfacial thickness, as functions of temperature and molecular characteristics of the substances, including molecular size and dispersive energy.